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Evaluation of the orientation relations from misorientation between inherited variants: Application to ausformed martensite

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Abstract—This paper describes a way to deduce the orientation relation occurring in phase transformation by only considering three misorientations between variants inherited from the same parent grain at a triple point. The method, named XABX, can be successfully applied even in materials deformed before phase transformation. This new approach, developed for investigating orientation relations in steels, is easily transposable for studying orientation relations of other phase transformations.

Keywords: Phase transformations; Variants; Orientation relation determination; Steels

1. Introduction

Phase transformations strongly influence the microstructures of materials and consequently their mechanical properties through the orientation relations (ORs) between parent and child phases and spatial arrangement of selected variants. Therefore, the knowledge of accurate characteristics of the phase transformations is important. In this framework, the most precise determination of the ORs allows us to investigate the phase transformation conditions and types. For example, in steel transformations, the ORs between austenite and the child phase can be different from the classical Nishiyama–Wassermann (NW) or Kurdjumov–Sachs (KS) ORs [1–7]. The direct determination of the ORs requires that a sufficient amount of the parent phase is retained at room temperature [1,2]. When this is not the case, the evaluation of the OR can be performed by considering the coincidence of high indices pole figures (PFs) of experimental and calculated data [3,4,8]. Using this procedure in a first step, Miyamoto et al. [8] presented a numerical method to evaluate the OR occurring in the steel phase transformation. Following a similar approach, an analytical method to determine the OR has also been proposed [9]. Until now, all methods operating without retained parent phase implicitly assume that the orientation is constant within the parent grain. However, in deformed materials, orientation gradients exist. In the presence of such orientation variations, the later methods do not correctly operate. The method presented here applies even when the later methods do not operate correctly. It uses the local misorientations between variants to deduce the OR between the vanished parent and the child phase. We have named this method XABX after the formulae which allow the problem to be solved. Two application examples are presented: one to validate the method on a synthetic microstructure, the other on ausformed martensite.

2. Working hypotheses and equations

In this section, we derive the equations that allow the determination of the OR under two hypotheses. These hypotheses are further discussed in Section 4.

Let us consider the parent grain whose boundaries are the bold line shown in Fig. 1. The orientation of a point located at r_i is characterized by a rotation matrix $[g_\gamma(r_i)]$. After complete transformation, this parent grain transforms into several spatial domains (variants) whose boundaries are the thin lines. The variant orientations are defined by rotation matrices $[g_\alpha(r_i)]$.

In general, the relation between the parent and the child orientations can be expressed by a product of rotation matrices:

$$[g_\alpha(r_i)] = [g_\gamma(r_i)][P(r_i)][\Delta g(r_i)][C(r_i)] \quad (1)$$

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in which $[P(r_i)]$ is one element of the n_P rotational symmetry elements of the parent phase, $[C(r_i)]$ one element of the n_C rotational symmetry elements of the child phase and the rotation $[\Delta g(r_i)]$ corresponds to the OR between the parent and the child phase at location r_i.

Let us now consider three points $[r_1, r_2, r_3]$ located at a triple point which belong to the same parent grain (Fig. 1). The links between parent and child orientations read:

$$\begin{aligned}
[g_\alpha(r_1)] &= [g_\gamma(r_1)][P(r_1)][\Delta g(r_1)][C(r_1)] \\
[g_\alpha(r_2)] &= [g_\gamma(r_2)][P(r_2)][\Delta g(r_2)][C(r_2)] \\
[g_\alpha(r_3)] &= [g_\gamma(r_3)][P(r_3)][\Delta g(r_3)][C(r_3)]
\end{aligned} \tag{2}$$

The first hypothesis we made is that the parent orientations do not vary (or only vary very slightly) across the variant boundaries:

$$[g_\gamma(r_1)] = [g_\gamma(r_2)] = [g_\gamma(r_3)] = [g_\gamma] \tag{3}$$

The constancy of $[g_\gamma]$ in the vicinity of a triple point allows Eqs. (2) to be combined so that $[g_\gamma]$ disappears.

After some easy manipulations, the following expressions can be found:

$$\begin{aligned}
[g_\alpha(r_2)]^{-1}[g_\alpha(r_1)] &= ([P_2][\Delta g(r_2)][C_2])^{-1}([P_1][\Delta g(r_1)][C_1]) \\
[g_\alpha(r_3)]^{-1}[g_\alpha(r_1)] &= ([P_3][\Delta g(r_3)][C_3])^{-1}([P_1][\Delta g(r_1)][C_1]) \\
[g_\alpha(r_2)]^{-1}[g_\alpha(r_3)] &= ([P_3][\Delta g(r_3)][C_3])^{-1}([P_2][\Delta g(r_2)][C_2])
\end{aligned} \tag{4}$$

At this stage, a second hypothesis is introduced. We assume that the local ORs remain close to each other and thus close to a mean OR:

$$[\Delta g(r_i)] \cong \overline{[\Delta g]}$$

This leads to a replacement of Eqs. (4) by:

$$\begin{aligned}
[g_\alpha(r_2)]^{-1}[g_\alpha(r_1)] &\cong ([P_2]\overline{[\Delta g]}[C_2])^{-1}([P_1]\overline{[\Delta g]}[C_1]) \\
[g_\alpha(r_3)]^{-1}[g_\alpha(r_1)] &\cong ([P_3]\overline{[\Delta g]}[C_3])^{-1}([P_1]\overline{[\Delta g]}[C_1]) \\
[g_\alpha(r_3)]^{-1}[g_\alpha(r_2)] &\cong ([P_3]\overline{[\Delta g]}[C_3])^{-1}([P_2]\overline{[\Delta g]}[C_2])
\end{aligned} \tag{5}$$

To simplify the notation we put $[P_1]\overline{[\Delta g]}[C_1] = \overline{[\Delta g']}$, which corresponds to an equivalent mean OR.

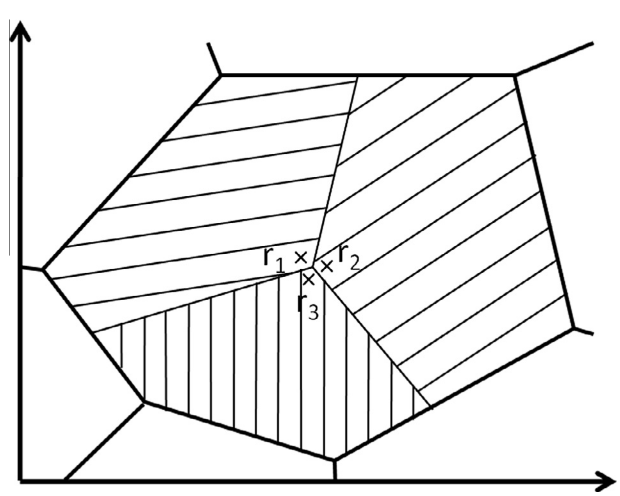

Fig. 1. The points of interest are located at a triple junction between three variants inherited from the same parent grain.

Then Eqs. (5) become:

$$\begin{aligned}
[g_\alpha(r_2)]^{-1}[g_\alpha(r_1)] &\cong ([P'_2]\overline{[\Delta g']}[C'_2])^{-1}\overline{[\Delta g']} \\
[g_\alpha(r_3)]^{-1}[g_\alpha(r_1)] &\cong ([P'_3]\overline{[\Delta g']}[C'_3])^{-1}\overline{[\Delta g']} \\
[g_\alpha(r_3)]^{-1}[g_\alpha(r_2)] &\cong ([P'_3]\overline{[\Delta g']}[C'_3])^{-1}\left([P'_2]\overline{[\Delta g']}[C'_2]\right)
\end{aligned} \tag{6}$$

which can be reformulated as:

$$\begin{aligned}
\overline{[\Delta g']}[C'_2][g_\alpha(r_2)]^{-1}[g_\alpha(r_1)] &\cong [P'_2]^{-1}\overline{[\Delta g']} \\
\overline{[\Delta g']}[C'_3][g_\alpha(r_3)]^{-1}[g_\alpha(r_1)] &\cong [P'_3]^{-1}\overline{[\Delta g']} \\
\overline{[\Delta g']}[C'_3][g_\alpha(r_3)]^{-1}[g_\alpha(r_2)][C'_2]^{-1} &\cong [P'_3]^{-1}[P'_2]\overline{[\Delta g']}
\end{aligned} \tag{7}$$

In this system, the inputs are the misorientations between three variants; the unknowns are $\overline{[\Delta g']}$ and the symmetry elements.

3. Orientation relation calculation

The general form of Eqs. (7) is $X \times A_i \cong B_i \times X$ (hence the name given to our the method) where A_i and B_i are functions of experimental data and of rotational symmetry elements and X stands for $\overline{[\Delta g']}$.

In this case, the mean local OR X, $\overline{[\Delta g']}$, must minimize the following error function:

$$E = \sum_i \|X \times A_i - B_i \times X\|^2 \tag{8}$$

with the constraint $\|X\|^2 = 1$ because X is a rotation matrix. In these expressions, $\|\|$ defines the Euclidean norm. The error function E is null if Eqs. (7) are equalities. But E may differ slightly from zero in the case of a small gradient of the parent orientation and/or in the case of variations of the local ORs.

The way to find out the value X which minimizes the error function E (Eq. (8)) is described in the Appendix. It passes through the use of quaternions whose properties are well adapted for this type of equation [10]. As shown in the Appendix A, the error function can be associated to a real positive (4×4) matrix whose components are function of the quaternions representing the rotations A_i and B_i. The four eigenvalues of this matrix (sorted from the largest: λ_1 to the smallest: λ_4) determine four values of the error function: λ_4 leads to the smallest value of Eq. (8) and its corresponding eigenvector stands for the OR X.

The symmetry elements P'_i and C'_i entering A_i and B_i are a priori not known. Therefore to find out X, we minimize the error function (Eq. (8)) for all combinations (C'_2, C'_3, P'_2, P'_3) of the n_P symmetry elements $[P_i]$ and n_C symmetry elements $[C_i]$. So the number of these calculations is $n_T = (n_C \times n_P)^2$.

Some data analysis is required to retain only the real OR among the n_T results. Let $\lambda_{4\min}$ be the minimum of the n_T λ_4s. All results having λ_4 close to $\lambda_{4\min}$ are potential solutions. If one of the potential solutions has λ_3 very close to λ_4, the system is underdetermined. In other words, it cannot be solved because at least two identical misorientations have been given as input data. If $\lambda_{4\min}$ is greater than $\lambda_{4\mathrm{CRIT}}$ then no OR relation exists within a given tolerance. The choice of $\lambda_{4\mathrm{CRIT}}$ is related to the deviation with which Eqs. (7) is respected; this is discussed in Section 4.

The potential solutions should be filtered because they contain symmetry equivalents of the OR. The remaining